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Structure at Calcite/Salt Solution Interfaces

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1 Introduction

Calcite, $CaCO_3$, is the main constituent of the natural materials chalk and limestone, which serve as hosts for oil reservoirs and drinking water aquifers. The affinity of the crystal surface for organic and water molecules, is critical for controlling the adsorption of toxic elements and desorption of oil molecules. Some salts dissolved in water might alter the affinity of the calcite surface. The salinity of NaCl in seawater is known to affect the wettability of chalk at high temperature, T at ~110°C [1]. Here we have measured the X-ray crystal truncation rod (CTR) profiles of calcite/NaCl(aq) interfaces, because the affinity can be interpreted by the atomic and thereby electronic structure at the interfaces.

2 Experiment

The structure of calcite is described by a rhombohedral cell containing two $CaCO_3$. The common cleavages become Miller-Bravais {10.4} in the hexagonal cell setting [2]. The surface of the freshly cleaved crystal was immersed in 0.5 mol/L NaCl solution. Just prior to the CTR measurements, the calcite was mounted on a thin-film liquid cell. The liquid cell was covered with a 7.5 μm-thick polyimide film to form a thin liquid film and prevent the solution from evaporating. The specular X-ray CTR scattering intensities for the {10.4} surface were measured at Photon Factory, KEK, Japan (BL-4C) by using monochromatic X-rays of 11.0 keV. The intensities were corrected for Lorentz, polarization, attenuation, and rod interception effects. The CTR profile was obtained in the range l = 0.5–11.8 with individual rocking scans at given {*hk.l*} values. In order to know the temperature effects on the interfacial structure, a new sample cell was developed. The sample was measured at 25 and 45°C.

3 Results and Discussion

The specular CTR profiles for T = 25 and 45°C are plotted in Fig. 1. The vertical axis indicates the absolute value of structure factor. The peaks at l = 4 and 8 correspond to the Bragg points of calcite (10.4) and (20.8). The intensity at the middle between the Bragg points reflects the scattering from the interface; therefore, the intensity in between Bragg points should be compared in order to reveal the difference of the structure at different temperature.

There was no significant difference between T = 25 and 45°C within the error. This indicates that the interfacial structure was not changed by the increased temperature. This result is consistent with the result that the wettability alteration by sea water gets significant at above 90°C [3].

In future experiments, we will measure the CTR profiles at higher temperatures and different salt concentrations to compare the response of the electron density profiles. The results will contribute to reveal the possibility of wettability modification by a salt dissolved in sea water.

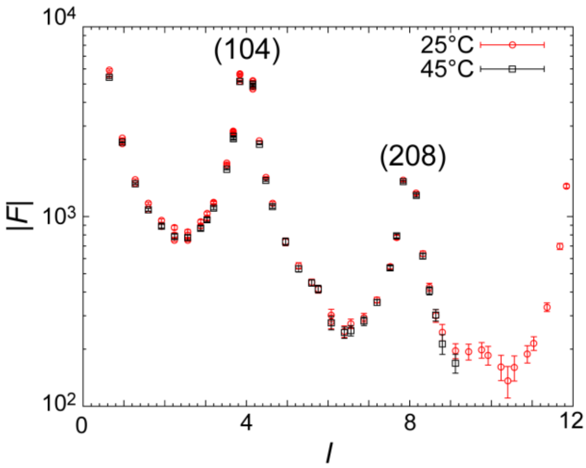

Fig. 1: X-ray CTR scattering profiles for calcite/NaCl solution interfaces at T = 25 and 45°C

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